



# Applications



## > Medical:

### Real-time, Non-invasive Breath Gas Analysis

#### REAL-TIME BREATH ANALYSIS

Breath gas analysis of volatile organic compounds (VOCs) has become a growing field of research in recent years. It is a non-invasive approach with many potential applications such as screening for diseases biomarkers, monitoring of metabolic processes, studying pharmacokinetics, and drug testing.

#### BENEFITS OF IONICON PTR-TOFMS

IONICON PTR-MS systems are powerful tools for breath gas analysis: Their detection limits and linearity range match the concentrations of breath VOCs. In addition, the high sensitivity and fast response time of IONICON PTR-MS systems allows to analyze breath online and in real-time. IONICON PTR-TOFMS record the complete spectra in a fraction of a second. Combined with their high mass resolving power several hundred compounds can be detected from a single exhalation.

#### BET-med BREATH SAMPLING INLET

IONICON has developed a specialized breath sampling inlet for PTR-MS. This Buffered End-Tidal Breath sampler (BET-med) uses inert and heated surfaces to avoid condensation, and can be used with commercial single-use mouthpieces. Most importantly, it is certified for medical use (ISO 60601) and allows real-time breath analysis in a clinical setting.

## PTR-MS

- > Real-time breath analysis
- > Screening for disease markers
- > Ultra-low detection limits (pptv)
- > Certified for clinical use (ISO 60601)

Find out more:

[www.ionicon.com/medical](http://www.ionicon.com/medical)



## SCREENING FOR BREATH MARKERS

The classical application is the search for breath biomarkers. In such screening studies, breath spectra of healthy volunteers are compared to subjects/patients with a certain condition. IONICON PTR-TOFMS instruments are particularly well suited, since the complete spectrum is analyzed at once [1].

The most prominent breath markers are those for smoking, which can therefore be used to benchmark the method. With PTR-MS we reach a cross-validated accuracy (AUROC) of 99%, which represents the best value published so far for a large study [2].

## LUNG CANCER MARKERS

In a multi-centric clinical study we could identify biomarkers for lung cancer. By combining only two markers, we reach a cross-validated AUROC value of > 83% for the detection of bronchial adeno-carcinoma [3].

## MONITORING STUDIES

Real-time breath analysis enabled new types of studies, where the breath of a subject is monitored to follow the variation of one or several marker compounds in time. In these monitoring studies the subjects act as their own control, which facilitates data interpretation greatly.

## PHARMACOKINETICS

The study of distribution and elimination of drugs in the body is called Pharmacokinetics. With breath analysis, the blood concentration of a drug can be monitored non-invasively and is updated with every exhalation. In the figure, the drug concentration shows a sharp increase and a slow decay from which pharmacokinetic models can be derived. This behavior requires a high sampling frequency, which would be next to impossible with offline analysis or blood tests [4].

## MONITORING METABOLIC EFFECTS

Most volatile breath compounds play a role in several metabolic processes. By administering isotopically labelled educts, their metabolic products will also be labelled and can clearly be distinguished in a mass spectrum. This allows to probe and study specific metabolic processes and deficiencies, and opens the door to personalized medicine [5].

■ Sources:

- [1]: Herbig J, J Breath Res, vol. 3, no. 2, IOP, pp. 027004 (2009)
- [2]: Herbig J, 4th Int. Conf. on PTR-MS, IUP Conf. Series, pp. 46-50 (2009)
- [3]: Herbig J, 5th Int. Conf. on PTR-MS, IUP Conf. Series, pp. 31-33 (2011)
- [4]: Beauchamp J, J Breath Res, vol. 4, no. 2, IOP, pp. 026006 (2010)
- [5]: Winkler K, J Breath Res, vol. 7, no. 3, IOP, pp. 036006 (2013)

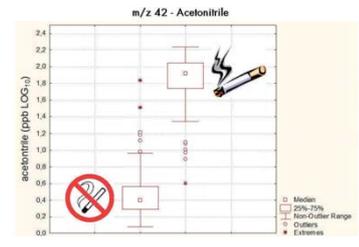


Fig. 1: Analyzing the breath of more than 200 subjects, several markers for smoking can be isolated. Most prominently acetonitrile, which leads to an almost perfect separation of smokers and non-smokers.

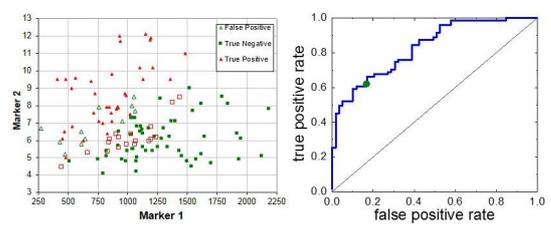


Fig. 2: Breath markers for lung cancer require a careful analysis of the data. We found two robust markers that give an AUROC value of > 83% (cross-validated).

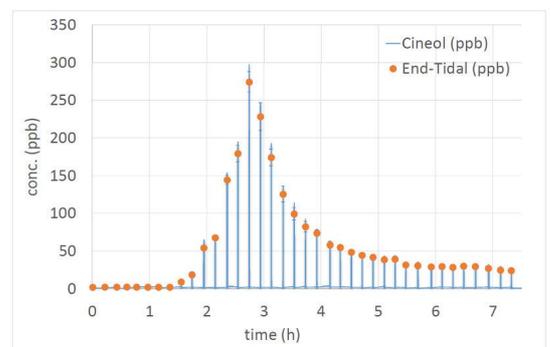


Fig. 3: Pharmacokinetic study: full exhalations, recorded every 15 minutes, which depicts the concentration of a drug in the exhaled breath after ingestion (t=0).

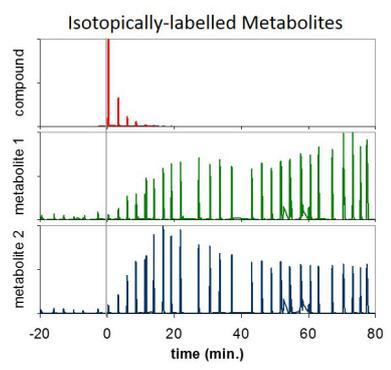


Fig. 4: Two isotopically labelled metabolites (green, blue) with individual variations over time, which arise as a result of the ingestion of a labelled compound (red).